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Editorial

Special Issue on Advanced Computational Algorithms: Introduction

Many complex problems arising in different areas of science and engineering can be successfully studied by applying large scale mathematical models. Several important tasks have to be performed both during the development of a large scale mathematical model and during its application in the attempts to get answers to important questions related to the problems studied. The successful completion of the following tasks is crucial:

1. The developers have to decide how features of the physical or social problems studied can be described mathematically.
2. Efficient numerical methods have to be applied in order to represent the continuous mathematical models in a discrete form.
3. Enormous sets of input data have to be prepared and used.
4. The discrete systems of equations have to be treated using computers.
5. The output data calculated during the computer handling of the mathematical models have to be visualized and animated.
6. The reliability of the numerical results produced (by the computer program) has to be investigated.

The performing of **the first of these six tasks** will very often result in a system of partial differential equations (PDEs). It is important to check whether the properties of the problem studied are preserved in the developed mathematical model. It must be stressed here that as a rule many assumptions have to be made both because some properties of the studied problem are unknown and because an attempt to take into account all known properties of the problem will result in a very complex mathematical model. In the latter case, it will not be possible to treat the resulting mathematical model successfully, i.e. to complete the remaining five tasks.

The efficient completion of **the second task** is often very crucial. Many large scale mathematical models can be treated on the computers available (including here also powerful parallel architectures with up to thousands of processors) if and only if the best-suited numerical methods are selected and carefully implemented in sufficiently efficient codes (computer programs).

The third task is very often underestimated by the developers. However, it does not make any sense to develop a perfect mathematical model and to handle it with the most efficient numerical methods (i.e. to deal very successfully with the first two tasks) if it will not be possible to supply reliable input data for the required simulations and experiments. Very often it is difficult to find the needed input data. Moreover, it is much more difficult to evaluate

(a) the reliability of the input data

as well as

(b) the effect of the uncertainties of the available input data on the model results.

Very often it is extremely difficult to handle the mathematical models on computers. The discrete systems often contain many millions of equations. Huge sets of input and output data must be stored in the computer. Therefore, there arise problems both with the storage needed and with the computing time used when the required simulations are to be carried out. It is not uncommon to find that the problems cannot be handled on the available computers. This means that **the fourth task** can also cause great problems. This is discussed in detail in the book of Zlatev and Dimov [1] for the case where environmental models are studied, but most of the conclusions that are drawn in this book are also applicable for many other large scale mathematical models.

The next difficulties arise very often when the first four tasks have been successfully completed. The computer will produce huge sets of output data and the developers have to deal with **the fifth task**. This means that the developers have to find out what information is hidden behind millions and millions of numbers calculated by the computer. It is amazing that the difficulties, which are related to the understanding of the meaning of the information contained in the enormous sets of output data, were foreseen about fifty years ago, in 1962, by Hamming [2]. At that time the output data files were

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much, much smaller than those appearing at present and in most cases it was not difficult at all to understand the meaning of the numbers calculated by the computers. Nevertheless, Hamming declared boldly and many times in his book "Numerical Methods for Scientists and Engineers" that

"The purpose of computing is insight, not numbers".

However, finding what the numbers are telling us became a real challenge, one of the greatest challenges, only in the new millennium.

After the achieving of the first five tasks, the developers have to answer at least two important questions:

(a) how big the uncertainties in the results obtained are

and

(b) what kind of question can be answered by using the calculated results.

This is **the sixth task** and it is also very challenging. There are several reasons for the appearance of uncertainties in the final results:

- The transition from the original physical or social problem to the mathematical problem often causes difficulties because some simplifying assumptions are unavoidable and are always made.
- The application of numerical methods causes both truncation errors and round-off errors in the output results. However, the use of more accurate numerical methods and double precision during the calculations will reduce these errors.
- The input data are nearly always (at least when the problems that are to be studied are very large and complicated) uncertain and it is very difficult to evaluate how big the uncertainties of these data are.

The short discussion of the difficulties sketched above shows clearly that it is very important to think carefully, *before the beginning of the solution of the problem studied* about the answer of the following question: *how will the results obtained in the solution be used?* The right answer to this question may lead to saving a lot of unnecessary effort. This conclusion is, of course, not something new. Such a requirement for the scientists who have to develop and to work with large scale mathematical models was also formulated in the book of Hamming [2].

The papers in this **Special Issue** are mainly devoted to the efficient solutions related to the second task. The tasks related to the improvement of the numerical methods as well as to the development of new and more efficient numerical methods remain extremely important for numerical analysts. The selected papers deal with the following important topics:

- Finite element methods applied in the discretization of several kinds of PDEs or systems of PDEs.
- Algebraic multilevel iterations applied in the solution of large systems of linear algebraic equations arising after the discretization of elliptic PDEs.
- Sensitivity analysis of the results obtained in the treatment of large scale air pollution models due to variation of the rates of different reactions in atmospheric chemical schemes.
- Using domain decomposition with preconditioning in the treatment of two-dimensional multi-body contact problems.
- Application of Galerkin projection methods in the numerical treatment of hyperbolic PDEs.
- Implementation of global and local nested mesh refinements.
- Treatment of non-homogeneous boundary conditions in the numerical solution of linear elliptic equations.
- Solution of some inverse problems for coefficient identification in the Euler–Bernoulli equation.
- Operator splitting and time stepping for the unsteady and incompressible Navier–Stokes equations.
- The transition of a continuous maximum principle to discrete schemes in connection with some parabolic PDEs.
- Application of some numerical methods in the numerical treatment of epidemiological models.
- Algorithms for preservation of non-negativity applied to problems arising after the discretization of two-dimensional heat conduction equations defined on a rectangular domain.
- Improving the accuracy of some numerical methods by using Richardson extrapolation and studying the stability properties of the combination of the θ-method and the Richardson extrapolation.

If the developers of large scale mathematical models are not interested in developing special numerical methods, and many scientists and engineers are certainly not willing to do this, then they must have a sufficiently large selection of numerical methods which can be used in their particular case. In such a case, they will be able to select the numerical method which is suitable for their model. The papers in the Special Issue "Advanced Computational Methods" will certainly contribute to the selection of promising numerical methods.

The papers in this issue were presented at the International Conference on Large Scale Scientific Computations held in June 4–8, 2009 (Sozopol, Bulgaria). The conferences on Large Scale Scientific Computers are held regularly, in every second year. The last conference was the seventh one. The next conference will presumably be held in June 2011. Sozopol is a very nice and quiet small town on the coast of the Black Sea and normally more than a hundred participants from many countries attend the conferences. We advise the readers of this Special Issue to consider the possibility of attending the next conference in Sozopol.

We, the guest-editors of this Special Issue, would like to thank very much the authors of all papers for

- agreeing to submit their papers,
- carefully reading the comments of the referees

and

- re-submitting the corrected papers in time.

Finally, we should like to thank very much the Editorial Board of the Journal of Computational and Applied Mathematics and especially Professor Wuytack for the kind permission to prepare this Special Issue on Advanced Computational Methods.

References

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[2] R.W. Hamming, Numerical Methods for Scientists and Engineers, McGraw-Hill, New York, San Francisco, Toronto, London, 1962.

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